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Model-based integration of enantiomer and stable isotope fractionation for chiral pesticides degradation

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Understanding the environmental distribution and the degradation processes of chiral pesticides is essential for risk assessment and for evaluating the hazardous effects of these organic compounds in both wastewater treatment systems and natural aquatic environments (Wong, 2006). The combination of stable isotope and enantiomer analysis techniques has been recently proposed to better characterize the fate of chiral pesticides. Different reaction pathways are characterized and effectively visualized by plotting enantiomer ratios together with stable isotope ratios.

First-principle based numerical modeling is an important tool to describe the evolution of concentration and isotope data during contaminant degradation (Aeppli et al., 2009), as well as to provide a quantitative description of different reaction pathways (Jin & Rolle, 2014). In this study, we introduce a modeling approach with the aim of unifying and integrating the interpretation of isotopic and enantiomeric fractionation. The model is based on the definition of enantiomer-specific isotopologues and jointly predicts the evolution of concentration, enantiomer fractionation, as well as changes in stable isotope ratios of different elements. The method allows evaluating different transformation pathways and was applied to investigate enzymatic degradation of dichlorprop (DCPP), enzymatic degradation of mecoprop methyl ester (MCPPM), and microbial degradation of α -hexachlorocyclohexane (α -HCH) by different bacterial strains and under different redox conditions. The proposed modeling approach was tested and validated with isotopic and enantiomeric data observed in previous experimental studies (Bashir et al., 2013; Jammer et al., 2014; Qiu et al., 2014). The model results reproduce the observed isotope and enantiomer ratios and precisely capture the dual-dimensional trends characterizing different reaction pathways. Furthermore, the model allows testing possible combinations of enantiomer analysis (EA), compound specific isotope analysis (CSIA), and enantiomer specific isotope analysis (ESIA) to identify and assess isotope and enantiomer selective reaction mechanisms.

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